

A New Approach of Deriving Bounds between Entropy and Error from Joint Distribution: Case Study for Binary Classifications

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Abstract—The existing upper and lower bounds between entropy and error are mostly derived through an inequality means without linking to joint distributions. In fact, from either theoretical or application viewpoint, there exists a need to achieve a complete set of interpretations to the bounds in relation to joint distributions. For this reason, in this work we propose a new approach of deriving the bounds between entropy and error from a joint distribution. The specific case study is given on binary classifications, which can justify the need of the proposed approach. Two basic types of classification errors are investigated, namely, the Bayesian and non-Bayesian errors. For both errors, we derive the closed-form expressions of upper bound and lower bound in relation to joint distributions. The solutions show that Fano's lower bound is an exact bound for any type of errors in a relation diagram of "Error Probability vs. Conditional Entropy". A new upper bound for the Bayesian error is derived with respect to the minimum prior probability, which is generally tighter than Kovalevskij's upper bound.

Index Terms—Entropy, error probability, Bayesian errors, analytical, upper bound, lower bound

I. INTRODUCTION

In information theory, the relations between entropy and error probability are one of the important fundamentals. Among the related studies, one milestone is Fano's inequality (also known as Fano's lower bound on the error probability of decoders), which was originally proposed in 1952 by Fano, but formally published in 1961 [1]. It is well known that Fano's inequality plays a critical role in deriving other theorems and criteria in information theory [2][3][4]. However, within the research community, it has not been widely accepted exactly who was first to develop the upper bound on the error probability [5]. According to [6] [7], Kovalevskij [8] was recognized as the first to derive the upper bound of the error probability in relation to entropy in 1965. Later, several researchers, such as Chu and Chueh in 1966 [9], Tebbe and Dwyer III in 1968 [10], Hellman and Raviv in 1970 [11], independently developed upper bounds.

The upper and lower bounds of error probability have been a long-standing topic in studies on information theory [12] [13] [14] [15] [16] [18] [19] [20][6] [7][21]. However, we consider two issues that have received less attention in these studies:

- I. What are the closed-form relations between each bound and joint distributions in a diagram of entropy and error probability?
- II. What are the lower and upper bounds in terms of the non-Bayesian errors if a non-Bayesian rule is applied in the information processing?

The first issue implies a need for a complete set of interpretations to the bounds in relation to joint distributions, so that both error probability and its error components are known for interpretations. We will discuss the reasons of the need in the later sections of this paper. Up to now, most existing studies derived the bounds through an inequality means without using joint distribution information. Therefore, their bounds are not described by a generic relation to joint distributions. Using the truncated-distribution approach, a significant study by Ho and Verdú [21] was reported recently on established the relations for general cases of variables with finite alphabets and countably infinite alphabets. Regarding the second issue, to our best knowledge, it seems that no study is shown in open literature on the bounds in terms of the non-Bayesian errors. We will define the Bayesian and non-Bayesian errors in Section III. The non-Bayesian errors are also of importance because most classifications are realized within this category.

The issues above form the motivation behind this work. We take binary classifications as a problem background since it is more common and understandable from our daily-life experiences. Moreover, we intend to simplify settings within a binary state and Shannon entropy definitions for a case study from an expectation that the central principle of the approach is well highlighted by simple examples. The novel contribution of the present work is given from the following three aspects:

- I. A new approach is proposed for deriving bounds directly through the optimization process based on a joint distribution, which is significantly different from all other existing approaches. One advantage of using the approach is a possible solution of closed-form expressions to the bounds.
- II. A new upper bound in a diagram of "Error Probability vs. Conditional Entropy" for the Bayesian errors is derived with a closed-form expression in the binary state, which is not reported before. The new bound is generally tighter than Kovalevskij's upper bound.
- III. The comparison study on the bounds in terms of the Bayesian and non-Bayesian errors are made in the binary state. The connections of bounds are explored for a first

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time between two types of errors.

In the first aspect, we also conduct the actual derivation using a symbolic software tool, which presents a standard and comprehensive solution in the approach. The rest of this paper is organized as follows. In Section II, we present related works on the bounds. For a problem background of binary classifications, several related definitions are given in Section III. The bounds are given and discussed for the Bayesian and non-Bayesian errors in Sections IV and V, respectively. Interpretations to some key points are presented in Section VI. Finally, in Section VII we conclude the work and present some discussions. The source code from using symbolic software for the derivation is included in Appendixes A and B.

II. RELATED WORKS

Two important bounds are introduced first, which form the baselines for the comparisons with the new bounds. They were both derived from inequality conditions [1][8]. Suppose the random variables X and Y representing input and output messages (out of m possible messages), and the conditional entropy $H(X|Y)$ representing the average amount of information lost on X when given Y . Fano's lower bound [1] is given in a form of:

$$H(X|Y) \leq H(P_e) + P_e \log_2(m-1), \quad (1)$$

where P_e is the *error probability* (sometimes, also called *error rate* or *error* for short), and $H(P_e)$ is the binary entropy function defined by [22]:

$$H(P_e) = -P_e \log_2 P_e - (1 - P_e) \log_2 (1 - P_e). \quad (2)$$

The base of the logarithm is 2 so that the units are *bits*.

The upper bound is given by Kovalevskij [8] in a piecewise linear form [10]:

$$H(X|Y) \geq \log_2 k + k(k+1) \left(\log_2 \frac{k+1}{k} \right) \left(P_e - \frac{k-1}{k} \right), \quad \text{and } k < m, m \geq 2, \quad (3)$$

where k is a positive integer number, but defined to be smaller than m . For a binary classification ($m = 2$), Fano-Kovalevskij bounds become:

$$H^{-1}(P_e) \leq P_e \leq \frac{H(X|Y)}{2}, \quad (4)$$

where $H^{-1}(P_e)$ is an inverse of $H(P_e)$. Feder and Merhav [23] depicted bounds of eq. (4) and presented interpretations on the two specific points from the background of data compression problems.

Studies from the different perspectives have been reported on the bounds between error probability and entropy. The initial difference is made from the entropy definitions, such as Shannon entropy in [12][14][24][25], and Rényi entropy in [15][6][7]. The second difference is the selection of bound relations, such as " P_e vs. $H(X|Y)$ " in [12][23], " $H(X|Y)$ vs. P_e " in [14] [15][6][7][21], " P_e vs. $MI(X, Y)$ " in [26][27], and " $NMI(X, Y)$ vs. A " in [24], where A is the accuracy rate, $MI(X, Y)$ and $NMI(X, Y)$ are the mutual information and normalized mutual information between variables X and Y , respectively. Another important study is made on the tightness

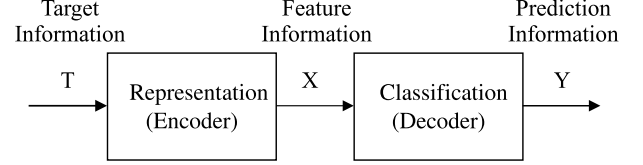


Fig. 1. Schematic diagram of the pattern recognition systems (modifications on FIGURE 1.7 in [29]).

of bounds. Several investigations [17] [18] [20] [21] have been reported on the improvement of bound tightness. Recently, a study in [25] suggested that an upper bound from the Bayesian errors should be added, which is generally neglected in the bound analysis.

III. BINARY CLASSIFICATIONS AND RELATED DEFINITIONS

Classifications can be viewed as one component in pattern recognition systems [29]. Fig. 1 shows a schematic diagram of the pattern recognition systems. The first unit in the systems is termed *representation* in the present problem background, but called *encoder* in communication background. This unit processes the tasks of *feature selection*, or *feature extraction*. The second unit is called *classification* or *classifier* in applications. Three sets of variables are involved in the systems, namely, *target variable* T , *feature variables* X , and *prediction variable* Y . While T and Y are univariate discrete random variables for representing labels of the samples, X can be high-dimension random variables either in forms of discrete, continuous, or their combinations.

In this work, binary classifications are considered as a case study because they are more fundamental in applications. Sometimes, multiclass classifications are processed by binary classifiers [28]. In this section, we will present several necessary definitions for the present case study. Let \mathbf{x} be a random sample satisfying $\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^d$, which is in a d -dimensional feature space and will be classified. The true (or target) state t of \mathbf{x} is within the finite set of two classes, $t \in \mathcal{T} = \{t_1, t_2\}$, and the prediction (or output) state $y = f(\mathbf{x})$ is within the two classes, $y \in \mathcal{Y} = \{y_1, y_2\}$, where f is a function for classifications. Let $p(t_i)$ be the *prior probability* of class t_i and $p(\mathbf{x}|t_i)$ be the *conditional probability density function* (or *conditional probability*) of \mathbf{x} given that it belongs to class t_i .

Definition 1: (Bayesian error in binary classification) In a binary classification, the *Bayesian error*, denoted by P_e , is defined by [29]:

$$P_e = \int_{R_2} p(t_1|\mathbf{x})p(t_1)d\mathbf{x} + \int_{R_1} p(t_2|\mathbf{x})p(t_2)d\mathbf{x}, \quad (5)$$

where R_i is the *decision region* for class t_i . The two regions are determined by the Bayesian rule:

$$\begin{aligned} \text{Decide } R_1 & \text{ if } \frac{p(\mathbf{x}|t_1)p(t_1)}{p(\mathbf{x}|t_2)p(t_2)} \geq 1, \\ \text{Decide } R_2 & \text{ if } \frac{p(\mathbf{x}|t_1)p(t_1)}{p(\mathbf{x}|t_2)p(t_2)} < 1, \end{aligned} \quad (6)$$

In statistical classifications, the Bayesian error is the *theoretically lowest* probability of error [29].

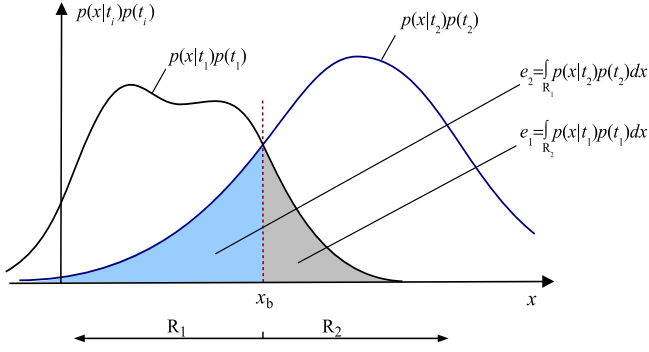


Fig. 2. Bayesian decision boundary x_b for equal priors $p(t_i)$ in a binary classification (modifications on FIGURE 2.17 in [29]).

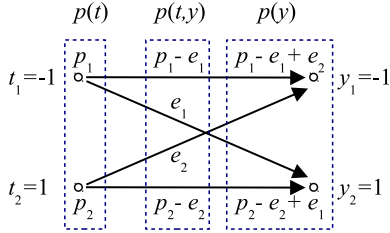


Fig. 3. Graphic diagram of the probability transformation between variables T and Y in a binary classification.

Definition 2: (Non-Bayesian error) The *non-Bayesian error*, denoted by P_E , is defined to be any error which is larger than the Bayesian error, that is:

$$P_E > P_e, \quad (7)$$

for the given information of $p(t_i)$ and $p(\mathbf{x}|t_i)$.

Remark 1: Based on the definitions above, for the given joint distribution the Bayesian error is unique, but the non-Bayesian errors are multiple. Fig. 2 shows the Bayesian *decision boundary*, x_b , on a univariate feature variable x for equal priors. The Bayesian error is $P_e = e_1 + e_2$. Any other decision boundary different from x_b will generate the non-Bayesian error for $P_E > P_e$.

In a binary classification, the *joint distribution*, $p(t, y) = p(t = t_i, y = y_j) = p_{ij}$, is given in a general form of:

$$\begin{aligned} p_{11} &= p_1 - e_1, & p_{12} &= e_1, \\ p_{21} &= e_2, & p_{22} &= p_2 - e_2, \end{aligned} \quad (8)$$

where $p_1 = p(t_1)$ and $p_2 = p(t_2)$ are the prior probabilities of Class 1 and Class 2, respectively; their associated errors (also called *error components*) are denoted by e_1 and e_2 . Fig. 3 shows a graphic diagram of the probability transformation between target variable T and perdition variable Y via their joint distribution $p(t, y)$ in a binary classification. The constraints in eq. (8) are given by [29]:

$$\begin{aligned} 0 < p_1 < 1, & \quad 0 < p_2 < 1, & \quad p_1 + p_2 &= 1 \\ 0 \leq e_1 \leq p_1, & \quad 0 \leq e_2 \leq p_2. \end{aligned} \quad (9)$$

In this work, we use e to denote error probability, or error variable, for representing either the Bayesian error or non-

Bayesian error. They are calculated from the same formula:

$$e(P_e, \text{ or } P_E) = e_1 + e_2. \quad (10)$$

Definition 3: (Minimum and maximum error bounds in binary classifications) Classifications suggest the minimum error bound as:

$$(P_E)_{\min} = (P_e)_{\min} = 0, \quad (11)$$

where the subscript *min* denotes the minimum value. The maximum error bound for the Bayesian error in binary classifications is [25]:

$$(P_e)_{\max} = p_{\min} = \min\{p_1, p_2\}, \quad (12)$$

where the symbol *min* denotes a *minimum* operation. For the non-Bayesian error, its maximum error bound becomes

$$(P_E)_{\max} = 1. \quad (13)$$

Remark 2: For a given set of joint distributions in the bound studies, one may fail to tell if it is the solution from using the Bayesian rule or not. For simplification, we distinguish the set to be one for the Bayesian errors if an error rate e always satisfies the relation of $e \leq p_{\min}$. Otherwise, it is a set for the non-Bayesian errors.

In a binary classification, the *conditional entropy*, $H(T|Y)$, is calculated from the joint distribution in (8):

$$\begin{aligned} H(T|Y) &= H(T) - MI(T, Y) \\ &= -p_1 \log_2 p_1 - p_2 \log_2 p_2 \\ &\quad - e_1 \log_2 \frac{e_1}{(p_2 + e_1 - e_2)p_1} \\ &\quad - e_2 \log_2 \frac{e_2}{(p_1 - e_1 + e_2)p_2} \\ &\quad - (p_1 - e_1) \log_2 \frac{(p_1 - e_1)}{(p_1 - e_1 + e_2)p_1} \\ &\quad - (p_2 - e_2) \log_2 \frac{(p_2 - e_2)}{(p_2 + e_1 - e_2)p_2}, \end{aligned} \quad (14)$$

where $H(T)$ is a *binary entropy* of the random variable T , and $MI(T, Y)$ is *mutual information* between variables T and Y .

Remark 3: When a joint distribution $p(t, y)$ is given, its associated conditional entropy $H(T|Y)$ is uniquely determined. However, for the given $H(T|Y)$, it is generally unable to reach a unique solution to $p(t, y)$, but mostly multiple solutions shown later in this work.

Definition 4: (Admissible point, admissible set, and their properties in diagram of entropy and error probability) In a given diagram of entropy and error probability, if a point in the diagram is possibly to be realized from a non-empty set of joint distributions for the given classification information, it is defined to be an *admissible point*. Otherwise, it is a *non-admissible point*. All admissible points will form an *admissible set* (or *admissible region(s)*), which is enclosed by the bounds (also called *boundary*). If every point located on the boundary is admissible (or non-admissible), we call this admissible set *closed* (or *open*). If only a partial portion of boundary points is admissible, the set is said *partially closed*. For an admissible point with the given conditions, if it is realized only by a unique joint distribution, it is called a *one-to-one mapping* point. If more than one joint distribution is associated to the same admissible point, it is called a *one-to-many mapping* point.

We consider that classifications present an exemplary justification of raising the first issue in Section I about the bound studies. The main reason behind the issue is that a single index of error probability may not be sufficient for dealing with classification problems. For example, when processing class-imbalance problems [30][31], we need to distinguish *error types*. In other words, for the same error probability e (or even the same admissible point), we are required to know the error components of e_1 and e_2 as well. Suppose one encounters a medical diagnosis problem, where p_1 generally represents the *majority class* for *healthy* persons (labeled with *negative* or -1 in Fig. 3), and p_2 the *minority class* for *abnormal* persons (labeled with *positive* or 1). A class-imbalance problem is then formed. While e_1 (also called *type I error*) is tolerable, e_2 (or *type II error*) seems intolerable because abnormal persons are considered to be “*healthy*”. Hence, from either theoretical or application viewpoint, it is necessary for establishing relations between bounds and joint distributions, which can provide error type information within error probability for better interpretations to the bounds.

IV. UPPER AND LOWER BOUNDS FOR BAYESIAN ERRORS

In this work, we select the bound relations between entropy and error probability. Furthermore, The bounds and their associated error components are also given by the following two theorems in a context of binary classifications.

Theorem 1: (Lower bound and associated error components) The lower bound in a diagram of “ P_e vs. $H(T|Y)$ ” and the associated error components are given by:

$$P_e \geq \min\{0, G_1(H(T|Y))\}, \quad (15a)$$

$$\begin{aligned} \text{for } G_1^{-1}(P_e) &= H(T|Y) \\ &= -P_e \log_2 P_e - (1 - P_e) \log_2 (1 - P_e), \\ P_e &= e_1 + e_2 \leq p_{\min}, \end{aligned} \quad (15b)$$

$$(e_1, e_2) = \begin{cases} (0.5, 0) \text{ or } (0, 0.5), & \text{if } P_e = 0.5, \\ (\frac{P_e(1-p_1-P_e)}{1-2P_e}, \frac{P_e(p_1-P_e)}{1-2P_e}), & \text{otherwise,} \end{cases} \quad (15c)$$

where $H(T|Y)$ is the conditional entropy of T when given Y , and G_1 is called the *lower bound function* (or *lower bound*). However, one can only achieve the closed-form solution on its inverse function, $G_1^{-1}(\cdot)$, not on itself.

Proof: Based on eq. (14), the lower bound function is derived from the following definition:

$$\begin{aligned} G_1^{-1}(e) &= \arg \max_e H(T|Y), \\ &\text{subject to eqs. (9) and (10),} \end{aligned} \quad (16)$$

where we take e for the input variable in the derivations. Eq. (16) describes the function of the maximum $H(T|Y)$ with respect to e , and the function needs to satisfy the general constraints of joint distributions in eq. (9). $H(T|Y)$ seems to be governed by the four variables from p_i and e_i in eq. (14). However, only two independent parameter variables determine the solutions of (14) and (16). The variable reduction from four to two is due to the two specific constraints imposed between parameters, that is, $p_1 + p_2 = 1$ and $e_1 + e_2 = e$. When we

set p_1 and e_1 as two independent variables, eq. (16) is then equivalent to solving the following problem:

$$\begin{aligned} G_1^{-1}(p_1, e_1) &= \arg \max_{e=P_e} H(T|Y), \\ &\text{subject to eqs. (9) and (10).} \end{aligned} \quad (17)$$

$G_1^{-1}(p_1, e_1)$ is a continuous and differentiable function with respect to the two variables. A differential approach is applied analytically for searching the *critical points* of the optimizations in eq. (17). We achieve the two differential equations below and set them to be zeros:

$$\begin{cases} \frac{\partial H(T|Y)}{\partial e_1} = \log_2 \frac{(p_1-e_1)(P_e-e_1)(1+2e_1-p_1-P_e)^2}{e_1(1+e_1-p_1-P_e)(p_1+P_e-2e_1)^2} = 0, \\ \frac{\partial H(T|Y)}{\partial p_1} = \log_2 \frac{(p_1-2e_1+P_e)(1+e_1-p_1-P_e)}{(p_1-e_1)(1+2e_1-p_1-P_e)} = 0. \end{cases} \quad (18)$$

By solving them simultaneously, we obtain the three pairs of the critical points through analytical derivations:

$$\begin{cases} e_1 = \frac{P_e(1-p_1-P_e)}{1-2P_e}, \\ p_1 = \frac{P_e+2e_1P_e-e_1-P_e^2}{P_e}, \end{cases} \quad (19a)$$

$$\begin{cases} e_1 = \frac{p_1(p_1+P_e-1)}{2P_1-1}, \\ p_1 = \frac{1-P_e}{2} + e_1 + \frac{1}{2}\sqrt{1+P_e^2+4e_1^2-4e_1P_e-2P_e}, \end{cases} \quad (19b)$$

$$\begin{cases} e_1 = \frac{p_1(p_1+P_e-1)}{2P_1-1}, \\ p_1 = \frac{1-P_e}{2} + e_1 - \frac{1}{2}\sqrt{1+P_e^2+4e_1^2-4e_1P_e-2P_e}. \end{cases} \quad (19c)$$

The highest order of each variable, e_1 and p_1 , in eq. (18) is four. However, we can see the component within the first function in eq. (18), $(1+2e_1-p_1-P_e)^2$, will degenerate the total solution order from four to three. Therefore, the three pairs of critical points exhibit a complete set of *possible solutions* to the problem in eq. (17). The *final solution* should be the pair(s) that satisfies both the maximum $H(T|Y)$ with respect to e_1 for the given $e = P_e$ and the constraints. Due to high complexity of the nonlinearity of the second-order partial differential equations on $H(T|Y)$, it seems intractable to examine the three pairs analytically for the final solution.

To overcome the difficulty above, we apply a symbolic software tool, MapleTM9.5 (a registered trademark of Waterloo Maple, Inc.), for a *semi-analytical* solution to the problem (see Maple code in Appendix A). For simplicity and without loss of generality in classifications, we consider p_1 and P_e are known constants in the function. The concavity property of $H(T|Y)$ with respect to e_1 in the ranges defined in eq. (9) is confirmed numerically by varying data on p_1 and P_e . A single maximum solution on $H(T|Y)$ is always obtained, but it is described by the two sets of e_1 in (19) alternatively in different conditions of p_1 and P_e . ■

Remark 4: Theorem 1 achieves the same lower bound found by Fano [1] (Fig. 4), which is general for finite alphabets (or multiclass classifications). One specific relation to Fano’s bound is given by the *marginal probability* (see eq. (2-144) in [2]):

$$p(y) = (1 - P_e, \frac{P_e}{m-1}, \dots, \frac{P_e}{m-1}), \quad (20)$$

which is termed *sharp* for attaining equality in eq. (1) [2]. We call Fano’s bound an *exact* lower bound because every point on it is sharp. The sharp conditions in terms of error

components in (15c) are a special case of the study in [21], and can be derived directly from their Theorem 1.

Theorem 2: (Upper bound and associated error components) The upper bound and the associated error components are given by:

$$P_e \leq \min\{p_{\min}, G_2(H(T|Y))\}, \quad (21a)$$

$$\begin{aligned} \text{for } G_2^{-1}(e) &= H(T|Y) \\ &= -p_{\min} \log_2 \frac{p_{\min}}{P_e + p_{\min}} - P_e \log_2 \frac{P_e}{P_e + p_{\min}}, \end{aligned} \quad (21b)$$

$$\begin{aligned} \text{and } P_e &= e_1 + e_2 \leq p_{\min}, \\ e_i &= p_j, e_j = 0, p_i \geq p_j, i \neq j, i, j = 1, 2 \end{aligned} \quad (21c)$$

where G_2 is called the *upper bound function* (or *upper bound*). Again, the closed-form solution can be achieved only on its inverse function of $G_2^{-1}(\cdot)$.

Proof: The upper bound function is obtained from solving the following equation:

$$\begin{aligned} G_2^{-1}(p_1, e_1) &= \arg \min_{e=P_e} H(T|Y), \\ &\text{subject to eqs. (9) and (10).} \end{aligned} \quad (22)$$

Because the concavity property holds for $H(T|Y)$ with respect to e_1 for the constraints defined in eq. (9), the possible solutions of e_1 should be located at the two ending points of its feasible range, $(0, P_e)$. We can take the point which produces the smaller $H(T|Y)$ as the final solution. The solution from Maple code shown in Appendix B confirms the closed-form expressions in eq. (21). ■

Remark 5: Theorem 2 describes a novel set of upper bounds which is in general *tighter* than Kovalevskij's bound [8] for binary classifications (Fig. 4). For example, when $p_{\min} = 0.2$ is given, the upper bounds defined in eq. (21) shows a curve "O - C" plus a line "C - C'". Kovalevskij's upper bound, given by a line "O - C - A", is sharp only at Point O and Point C. The solution in eq. (21c) confirms an advantage of using the proposed optimization approach in derivations so that a closed-form expression of the exact bound is possibly achieved.

In comparison, Kovalevskij's upper bound described in eq. (3) is general for multiclass classifications. This bound misses a general relation to error components like eq. (21c), although the relation is restricted to a binary state. For distinguishing from the Kovalevskij's upper bound, we also call G_2 a *curved upper bound*. The new *linear upper bound*, $(P_e)_{\max} = p_{\min}$, shows the maximum error for the Bayesian decisions in binary classifications [25], which is also equivalent to the solution of a blind guess when using the maximum-likelihood decision [29]. If $p_1 = p_2$, the upper bound becomes a single curved one.

Remark 6: The lower and upper bounds defined by eqs. (15) and (21) form a closed admissible region in the diagram of " P_e vs. $H(X|Y)$ ". The shape of the admissible region changes depending on a single parameter of p_{\min} .

V. UPPER AND LOWER BOUNDS FOR NON-BAYESIAN ERRORS

In classification problems, the Bayesian errors can be realized only if one has the exact information about all probability

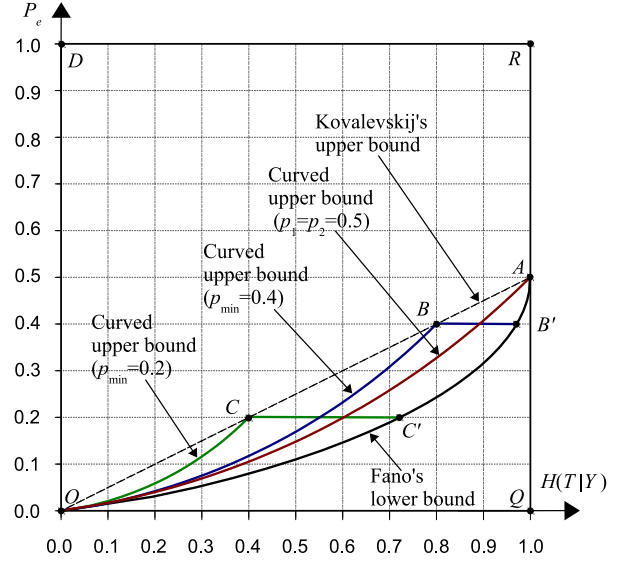


Fig. 4. Plot of bounds in a " P_e vs. $H(T|Y)$ " diagram.

distributions of classes. The assumption above is generally impossible in real applications. In addition, various classifiers are designed by employing the non-Bayesian rules, such as the conventional decision trees, artificial neural networks and supporting vector machines [29]. Therefore, the analysis of the non-Bayesian errors presents significant interests in classification studies.

Definition 5: (Label-switching in binary classifications) In binary classifications, a label-switching operation is an exchange between two labels. Suppose the original joint distribution is denoted by:

$$p_A(t, y) : \begin{aligned} p_{11} &= a, p_{12} = b, \\ p_{21} &= c, p_{22} = d. \end{aligned} \quad (23a)$$

A label-switching operation will change the prediction labels in Fig. 3 to be $y_1 = 1$ and $y_2 = -1$, and generate the following joint distribution:

$$p_B(t, y) : \begin{aligned} p_{11} &= b, p_{12} = a, \\ p_{21} &= d, p_{22} = c. \end{aligned} \quad (23b)$$

Proposition 1: (Invariant property from label-switching) The related entropy measures, including $H(T)$, $H(Y)$, $MI(T, Y)$, and $H(T|Y)$, will be invariant to labels, or unchanged from a label-switching operation in binary classifications. However, the error e will be changed to be $1 - e$.

Proof: Substituting the two sets of joint distributions in eq. (23) into each entropy measure formula respectively, one can obtain the same results. The error change is obvious. ■

Theorem 3: (Lower bound and upper bound for non-Bayesian error without information of p_1 and p_2) In a context of binary classifications, when information about p_1 and p_2 is unknown (say, before classifications), the lower bound and upper bound for the non-Bayesian error are given by:

$$G_1(H(T|Y)) \leq P_e \leq 1 - G_1(H(T|Y)), \quad (24a)$$

$$(e_1, e_2) = \begin{cases} (0.5, 0) \text{ or } (0, 0.5), & \text{if } p_1 = p_2 = P_E = 0.5, \\ \left(\frac{P_E(1-p_1-P_E)}{1-2P_E}, \frac{P_E(p_1-P_E)}{1-2P_E} \right), & \text{if } (1-p_1-P_E)(p_1-P_E)(P_E-0.5) > 0, \\ \left(\frac{p_1(p_1+P_E-1)}{2P_1-1}, \frac{(1-p_1)(p_1-P_E)}{2P_1-1} \right), & \text{otherwise,} \end{cases} \quad (24c)$$

$$\begin{aligned} \text{for } G_1^{-1}(P_E) &= H(T|Y) \\ &= -P_E \log_2 P_E - (1-P_E) \log_2 (1-P_E), \\ P_E &= e_1 + e_2 \leq 1, \end{aligned} \quad (24b)$$

$$(\text{see the top of this page}) \quad (24c)$$

where we call the upper bound in eq. (24a), $1 - G_1(H(T|Y))$, the *general upper bound* (or *mirrored lower bound*), which is a mirror of Fano's lower bound with the mirror axis along $P_E = 0.5$. Both bounds share the same expression for calculating the associated error components in eq. (24c). When $P_E \leq 0.5$, their components, e_1 and e_2 , correspond to the lower bound, otherwise, to the upper bound.

Proof: Suppose an admissible point is located at the lower bound which shows $P_E \leq 0.5$. By a label-switching operation, one can obtain the mirrored admissible point at $1 - P_E \geq 0.5$, which is located at the mirrored lower bound. Proposition 1 suggests both points share the same value of $H(T|Y)$. Because P_E is the smallest one for the given conditional entropy $H(T|Y)$, its mirrored point is the biggest one for creating the general upper bound. ■

Remark 7: Fano's lower bound, its mirror bound, and the axis of P_E form an admissible region, denoted by a boundary " $O - F' - A - F - D - O$ " in Fig. 5, for the non-Bayesian error when information about p_1 and p_2 is unknown. On the axis of P_E , only Points O and D are admissible. Hence, the admissible region is partially closed.

Theorem 4: (Admissible region(s) for non-Bayesian error with known information of p_1 and p_2) In binary classifications, when information about p_1 and p_2 is known, a closed admissible region for the non-Bayesian error is generally formed (Fig. 5) by Fano's lower bound, the general upper bound, the curved upper bound $G_2^{-1}(\cdot)$, the mirrored upper bound of $G_2^{-1}(\cdot)$, and the upper bound $H(T|Y)_{max}$. For the $H(T|Y)_{max}$ bound, its associated error components are given by:

$$\begin{aligned} \text{for } H(T|Y) &= H(T|Y)_{max} = H(e = p_{min}), \\ (e_1, e_2) &= \begin{cases} (0.25, 0.25), & \text{if } p_1 = p_2 = P_E = 0.5, \\ \left(\frac{p_1(1-p_1-P_E)}{1-2p_1}, \frac{P_E(1-p_1)-p_1(1-p_1)}{1-2p_1} \right), & \text{otherwise.} \end{cases} \end{aligned} \quad (25)$$

Proof: Following the proof in Theorem 3, one can get the mirrored upper bound of $G_2^{-1}(\cdot)$. The upper bound $H(T|Y)_{max}$ is calculated from the condition of $H(T|Y) \leq H(T)$ [2]. For the given p_1 and p_2 , $H(T|Y)_{max}$ is a constant. Because $H(T|Y)_{max}$ also implies a minimization of $MI(T, Y)$ in eq. (14), its associated error components can be obtained from the minimization relation of $MI(T, Y)$ in forms of (see eq. (35) in [33]):

$$\frac{p_{11}}{p_{21}} = \frac{p_{12}}{p_{22}}. \quad (26)$$

Remark 8: Eqs. (25) and (26) equivalently imply a zero value for the mutual information, $MI(T, Y) = 0$, which

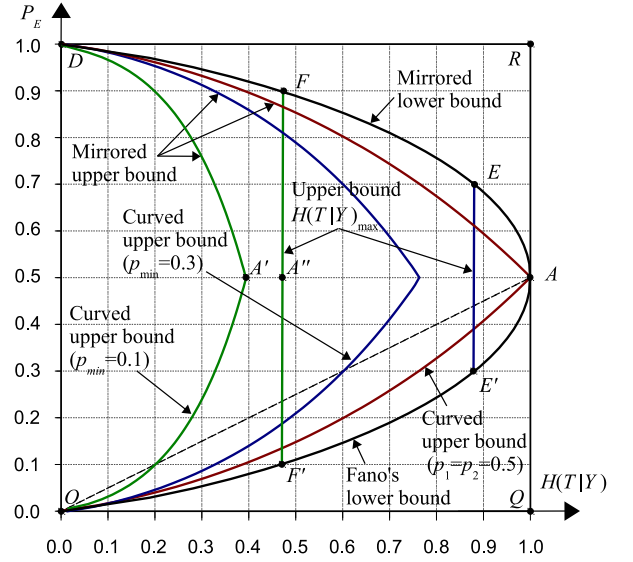


Fig. 5. Plot of bounds in a " P_E vs. $H(T|Y)$ " diagram.

suggests *no correlation* [29] or *statistically independent* [2] between two variables T and Y .

Remark 9: When information of p_1 and p_2 is known, the shape of the admissible region(s) is fully dependent on a single parameter p_{min} . Two closed admissible regions are formed only when $p_1 = p_2$ (Fig. 5). One region is from Fano's lower bound and the upper bound. The other is from the mirrored upper bound and the general upper bound. In general, the non-Bayesian error P_E can be higher than Kovalevskij's bound.

VI. CLASSIFICATION INTERPRETATIONS TO SOME KEY POINTS

For better understanding the theoretical results from a background of classifications, interpretations are given to some key points shown in Figs. 4 and 5, respectively. Those key points may hold special features in classifications.

Point O: This point represents a zero value of $H(T|Y)$. It also suggests a *perfect classification* without any error ($P_e = P_E = 0$) by a specific setting of the joint distribution:

$$\begin{aligned} p_{11} &= p_1, \quad p_{12} = 0, \\ p_{21} &= 0, \quad p_{22} = p_2. \end{aligned} \quad (27)$$

This point is always admissible and independent of error types.

Point A: This point shows the maximum ranges of $H(T|Y) = 1$ for *class-balanced* classifications ($p_1 = p_2$). Three specific classification settings can be obtained for representing this point. The two settings from eq. (24c) are actually *no classification*:

$$\begin{aligned} p_{11} &= 1/2, \quad p_{12} = 0, \text{ or } p_{11} = 0, \quad p_{12} = 1/2, \\ p_{21} &= 1/2, \quad p_{22} = 0, \quad p_{21} = 0, \quad p_{22} = 1/2. \end{aligned} \quad (28)$$

They also indicate *zero information* [32] from the classification decisions. The other setting is a *random guessing* from eq. (25):

$$\begin{aligned} p_{11} &= 1/4, & p_{12} &= 1/4, \\ p_{21} &= 1/4, & p_{22} &= 1/4. \end{aligned} \quad (29)$$

For the Bayesian errors, this point is always included by both Fanos' bound and Kovalevskij's bound. However, according to the upper bounds defined in (21a), this point is non-admissible whenever the relation of $p_1 = p_2$ does not hold. For the non-Bayesian errors, the point is either admissible or non-admissible depending on the given information about p_1 and p_2 . This example suggests that the admissible property of a point should generally rely on the given information in classifications.

Point D: This point occurs for the non-Bayesian classifications in a form of:

$$\begin{aligned} p_{11} &= 0, & p_{12} &= p_1, \\ p_{21} &= p_2, & p_{22} &= 0. \end{aligned} \quad (30)$$

In this case, one can exchange the labels for a perfect classification.

Point B: This point is located at the corner formed by the curved and linear upper bounds, with $H(T|Y) = 0.8$ and $e = 0.4$. In apart from Point *O*, this is another point obtained from eq. (21) that sets at Kovalevskij's upper bound. The point can be realized from either Bayesian or non-Bayesian classifications. Suppose $p_1 > p_2 = 0.4$ for the Bayesian classifications. One will achieve Point *B* by a classification:

$$\begin{aligned} p_{11} &= 0.2, & p_{12} &= 0.4, \\ p_{21} &= 0, & p_{22} &= 0.4, \end{aligned} \quad (31)$$

for a one-to-one mapping. In other words, the point becomes non-admissible whenever $p_{min} \neq 0.4$. If the non-Bayesian errors are considered, this point will possess a one-to-many mapping. For example, one can get another setting from solving $H(p_{min}) = 0.8$ for p_{min} first. Then, by substituting the relations of $p_2 = p_{min}$ and $P_E = 0.4$ into eq. (25), one can get the error components. The numerical results show the approximation solutions with $p_{min} \approx 0.2430$, $e_1 \approx 0.2312$, and $e_2 \approx 0.1688$ for another setting of Point *B*.

Point B': The point located at the lower bound, like Point *B'*, will produce a one-to-many mapping for either the Bayesian errors or non-Bayesian errors. One specific setting in terms of the Bayesian errors is:

$$\begin{aligned} p_{11} &= 0.6, & p_{12} &= 0, \\ p_{21} &= 0.4, & p_{22} &= 0, \end{aligned} \quad (32)$$

which suggests zero information from classifications. More settings can be obtained from eq. (15). For example, if given $p_1 = 0.55$, $p_2 = 0.45$ and $P_e = 0.4$, one can have:

$$\begin{aligned} p_{11} &= 0.45, & p_{12} &= 0.1, \\ p_{21} &= 0.3, & p_{22} &= 0.15. \end{aligned} \quad (33)$$

The non-Bayesian errors will enlarge the set of one-to-many mapping for an admissible point of the Bayesian errors due to the relaxed condition of (13). One setting is for the balanced error components:

$$\begin{aligned} p_{11} &= 0.3, & p_{12} &= 0.2, \\ p_{21} &= 0.2, & p_{22} &= 0.3. \end{aligned} \quad (34)$$

Eq. (24c) will be applicable for deriving a specific setting when p_1 and P_E are given. For example, two settings can be obtained:

$$\begin{aligned} \text{if} & & p_1 &= 0.25, & P_E &= 0.4, \\ \text{then} & & e_1 &= 0.175, & e_2 &= 0.225, \end{aligned} \quad (35)$$

$$\begin{aligned} \text{if} & & p_1 &= 0.3, & P_E &= 0.4, \\ \text{then} & & e_1 &= 0.225, & e_2 &= 0.175. \end{aligned} \quad (36)$$

for representing the same point, Point *B'*, which is located at $H(T|Y) \approx 0.9710$ and $P_E = 0.4$ in the diagram (Fig. 4).

Points E and E': All points located at the general upper bound, like Point *E*, will correspond to the settings from the non-Bayesian errors. If a point located at the lower bound, say *E'*, it can represent settings from either the Bayesian or non-Bayesian errors depending on the given information in classifications. Points *E* and *E'* form the mirrored points. Their settings can be connected by a relation in (23), but not a necessary. For example, one specific setting for Point *E'* with $p_1 = 0.3$ and $p_2 = 0.7$ is:

$$\begin{aligned} p_{11} &= 0, & p_{12} &= 0.3, \\ p_{21} &= 0, & p_{22} &= 0.7, \end{aligned} \quad (37)$$

the other for Point *E* with $p_1 = 0.8$ and $p_2 = 0.2$ is:

$$\begin{aligned} p_{11} &= \frac{20}{30}, & p_{12} &= \frac{4}{30}, \\ p_{21} &= \frac{9}{30}, & p_{22} &= \frac{1}{30}. \end{aligned} \quad (38)$$

They are mirrored to each other but have no label-switching relation.

Points A' and A'': When $P_E = 0.5$ and $p_{min} = 0.1$, Points *A'* and *A''* form a pair as the ending points for the given conditions. Supposing $p_1 = 0.9$ and $p_2 = 0.1$, one can get the specific setting for Point *A'* from eq. (21c):

$$\begin{aligned} p_{11} &= 0.4, & p_{12} &= 0.5, \\ p_{21} &= 0, & p_{22} &= 0.4, \end{aligned} \quad (39)$$

and one for Point *A''* from eq. (25):

$$\begin{aligned} p_{11} &= 0.45, & p_{12} &= 0.45, \\ p_{21} &= 0.05, & p_{22} &= 0.05. \end{aligned} \quad (40)$$

Points Q and R: The two points are specific due to their positions in the diagrams. For either type of errors, both points are non-admissible in the diagrams, because no setting exists in binary classifications which can represent the points.

VII. SUMMARY AND DISCUSSIONS

This work investigates into upper and lower bounds between entropy and error probability. An optimization approach is proposed to the derivations of the bound functions from a joint distribution. As a preliminary work, we consider binary classifications for a case study. Through the approach, a new upper bound is derived and shows tighter in general than Kovalevskij's upper bound. The closed-form relations between bounds and error components are presented. The analytical results lead to a better understanding about the sharp conditions of bounds in terms error components. Because classifications involve either Bayesian errors or non-Bayesian ones, we demonstrate the bounds comparatively for both types of errors.

We recognize that analytical tractability is an issue for the proposed approach. Fortunately, a symbolic software tool is helpful for solving complex problems successfully with different semi-analytical means (such as in [34][35]). The semi-analytical solution used in this work refers to the analytical derivation of possible solutions but the numerical verification of the final solution.

To emphasize the importance of the study, we present discussions below from the perspective of machine learning in big-data classifications. We consider that binary classifications will be one of key techniques to implement a *divide-and-conquer* strategy for efficiently processing large quantities of data. Class-imbalance problems with extremely-skewed ratios are mostly formed from a *one-against-other* division scheme for binary classes. Researchers, of course, concern error types in classification performance. The knowledge of bounds in relation to error components is desirable for theoretical and application purposes.

From a viewpoint of machine learning, the bounds derived in this work provide a basic solution to link learning targets between error and entropy in the related studies. *Error-based learning* is more conventional because of its compatibility with our intuitions in daily life, such as “*trial and error*”. Significant studies have been reported under this category. In comparison, *information-based learning* [36] is relatively new and uncommon in some applications, such as classifications. Entropy is not a well-accepted concept related to our intuition in decision making. This is one of the reasons why the learning target is chosen mainly based on error, rather than on entropy. However, we consider that error is an empirical concept, whereas entropy is theoretical and general. In [37], we demonstrated that entropy can deal with both notions of *error* and *reject* in abstaining classifications. Information-based learning [36] presents a promising and wider perspective for exploring and interpreting learning mechanisms.

When considering all sides of the issues stemming from machine learning studies, we believe that “*what to learn*” is a primary problem. However, it seems that more investigation is focused on the issue of “*how to learn*”, which should be put as the second-level problem. Moreover, in comparison with the long-standing yet hot theme of *feature selection*, little study has been done from the perspective of *learning target selection*. We propose that this theme should be emphasized in the study of machine learning. Hence, the relations studied in this work are fundamental and crucial to the extent that researchers, using either error-based or entropy-based approaches, are able to reach a better understanding about its counterpart.

ACKNOWLEDGMENTS

This work is supported in part by NSFC No. 61075051, SPRP-CAS No. XDA06030300 for BG, and NSFC No. 60903089 for HJ. The previous version of this work, entitled “Analytical bounds between entropy and error probability in binary classifications”, was appeared as arXiv:1205.6602v1[cs.IT] in May 30, 2012. Thanks to the anonymous reviewers for the comments and suggestions during the peer reviewing processing, particularly for our attention to the reference [21].

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APPENDIX A
MAPLE CODE FOR DERIVING THE LOWER BOUND

```

> restart;                                     # Clean the memory
> p2:=1-p1;e2:=Pe-e1;                         # Describe the bound with respect to p1 and e1
> HT:=-p1*log[2](p1)-p2*log[2](p2); # Shannon entropy
> p11:=(p1-e1);p12:=e1;p22:=p2-e2;p21:=e2;    # Terms of joint probability
> q1:=p11+p21;q2:=p12+p22;                   # Intermediate variables
> MI:=p11*log[2](p11/q1/p1)+p12*log[2](p12/q2/p1);
> MI=MI+p22*log[2](p22/q2/(1-p1))+p21*log[2](p21/q1/(1-p1)); # Mutual information
> HTY:=(HT-MI);                               # Conditional entropy
> HTY_dif_p1:=simplify(combine(diff(HTY,p1),ln, symbolic)); # Differential w.r.t. p1

$$\text{HTY\_dif\_p1} := \frac{\ln(2)}{\frac{\ln\left|\frac{(p1 - 2 e1 + Pe) (-1 + p1 + Pe - e1)}{(p1 - e1) (-2 e1 - 1 + p1 + Pe)}\right|}{2}}$$

> HTY_dif_e1:=simplify(combine(diff(HTY,e1),ln, symbolic)); # Differential w.r.t. e1

$$\text{HTY\_dif\_e1} := \frac{\ln(2)}{\frac{\ln\left|\frac{(p1 - e1) (-2 e1 - 1 + p1 + Pe) (Pe - e1)}{(p1 - 2 e1 + Pe) e1 (-1 + p1 + Pe - e1)}\right|}{2}}$$

> solve({HTY_dif_p1=0,HTY_dif_e1=0}, {e1, p1}); # not a complete set of
                                                    # possible solutions

$$< e1 = e1, p1 = -\frac{Pe^2 + e1 - Pe - 2 e1 Pe}{Pe} >$$

> E1:=solve(HTY_dif_e1, e1); # a complete set of possible solutions when p1 is known

$$E1 := \frac{Pe (-1 + p1 + Pe) p1 (-1 + p1 + Pe)}{2 Pe - 1}, \frac{2 p1 - 1}{2 Pe - 1}$$

> P1_a:=solve(E1[1]=e1, {p1});P1_bc:=solve(E1[2]=e1, {p1}); # a complete set of possible
                                                                # solutions when e1 is known

$$P1\_a := < p1 = -\frac{Pe^2 + e1 - Pe - 2 e1 Pe}{Pe} >$$


$$P1\_bc := < p1 = e1 + \frac{1}{2} - \frac{1}{2} Pe + \frac{1}{2} \sqrt{4 e1^2 - 4 e1 Pe + 1 - 2 Pe + Pe} >, \frac{(1/2)\sqrt{4 e1^2 - 4 e1 Pe + 1 - 2 Pe + Pe}}{2}$$


$$< p1 = e1 + \frac{1}{2} - \frac{1}{2} Pe - \frac{1}{2} \sqrt{4 e1^2 - 4 e1 Pe + 1 - 2 Pe + Pe} >$$

> simplify(combine(simplify(eval(HTY, e1=E1[1])),ln,symbolic)); # failed to show it explicitly
> simplify(eval(HTY, e1=E1[2])); # Display of the lower bound function in terms of p1

$$p1 \ln(p1) + \ln(1 - p1) - \ln(1 - p1) p1$$

<-----
ln(2)
> # verification of concavity of HTY by a numerical way (changing Pe and p1 arbitrarily
> Pe:=0.5;p1:=0.6;plot(HTY_graph,e1=0..Pe); # with the constraints)

```

APPENDIX B
MAPLE CODE FOR DERIVING THE UPPER BOUND

```

> restart;                                     # Clean the memory
> HT:=-p1*log[2](p1)-p2*log[2](p2);           # Shannon entropy
> p11:=(p1-e1);p12:=e1;p22:=p2-e2;p21:=e2;   # Terms of joint distribution
> # To examine the HTY on two ending points for e2, i.e., e2 = 0 and e2=e
> # For derivation of the upper bound function when e2=0
> e1:=e;e2:=0;p1:=1-p2;
> q1:=p11+p21;q2:=p12+p22;                   # Intermediate variables
> MI:=p11*log[2](p11/q1/p1)+p12*log[2](p12/q2/p1); # Mutual information
> MI:=MI+p22*log[2](p22/q2/(1-p1));           # Neglect one term when 0*log(0)=0
> HTY_1:=combine(simplify(combine(simplify(HT-MI),ln,symbolic)));
> # Display of the upper bound function when e2=e
      /e + p2\      /e + p2\
p2 ln|-----| + e ln|-----|
   \ p2  /       \ e  /
HTY_1 := -----
              ln(2)
> # For derivation of the upper bound function when e2=e
> e1:=0;e2:=e;
> q1:=p11+p21;q2:=p12+p22;                   # Intermediate variables
> MI:=p11*log[2](p11/q1/p1);                 # Neglect one term when 0*log(0)=0
> MI:=MI+p22*log[2](p22/q2/(1-p1))+p21*log[2](p21/q1/(1-p1));
> HTY:=eval(HT-MI,p2=1-P1);                  # Using P1 for p1
> HTY_2:=combine(simplify(combine(simplify(HTY),ln,symbolic)));
> # Display of the upper bound function in terms of e and p2
      / P1 \      / e \
-P1 ln|-----| - e ln|-----|
   \P1 + e/      \P1 + e/
HTY_2 := -----
              ln(2)
> # To calculate the difference between HTY_1 and HTY_2
> delta_HTY:=combine(simplify(HTY_1-HTY_2),ln,symbolic);
      /e + p2\      /e + p2\      / P1 \
p2 ln|-----| + e ln|-----| + P1 ln|-----|
   \ p2  /       \P1 + e/      \P1 + e/
delta_HTY := -----
              ln(2)
> # numerical verification of the solution to HTY below:
> # changing p2 arbitrarily with the constraint
> # when p2<0.5, delta_HTY<0, HTY_1 is the final solution,
> # when p2>0.5, delta_HTY>0, HTY_2 is the final solution,
> # when p2=0.5, delta_HTY=0, both are the solutions.
> p2:=0.4;P1:=1-p2;plot(delta_HTY,e=0..p2);

```